A probabilistic logic incorporating posteriors of hierarchic graphical models

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Motivation and background
Fusion of factual knowledge and complex posteriors
The „Most Probable Sentences” problem
Applications
Summary
Motivation

Background (e.g. biomedicine):
Rapidly accumulating heterogeneous data

Uncertain (statistical) sources
- Clinical observations
- Gene activity measurements
- Expert-defined models

Factual knowledge
- Domain ontologies
- Natural-language publications

Goal:
- Fusion
The model class: Bayesian networks

- directed acyclic graph (DAG)
  - nodes – domain entities
  - edges – direct probabilistic relations
- conditional probability models $P(X | Pa(X))$
- interpretations:

$$P(X_1, \ldots, X_N) = \prod_{i=1}^{N} P(X_i | Pa(X_i))$$

**DAG structure:** dependency map (d-separation)

**edges:** direct causal relations
Bayesian statistics and inference

Knowledge representation:
- set of models (feature values)
- distribution over them

Learning (predictive inference):
\[ P(G | D) = \frac{P(D | G) \times P(G)}{P(D)} \]

Parametric inference:
application: feature learning

\[ P(F = f) = \sum_{G:F^G = f} P(G) \]

- Practical methods: MCMC (Markov Chain Monte Carlo) sampling
Interesting Bayesian network features

Levels of model features/posteriors:
- full structures/DAGs
- Markov Blanket Graphs (MBGs)
  - (1) parents of the node,
  - (2) its children,
  - (3) parents of the children
- Markov Blankets (MBs)
  - the set of nodes which probabilistically isolate the target from the rest of the model
- Markov Blanket Membership (MBM)
- directed edges

Motivations:
- simpler (lower-level) features are easier to learn
Basics of MCMC methods I.

Goal:

- approximating the full-scale summation/integral with an average over DAGs

**DAG-MCMC algorithm:**

- random walk in the space of DAGs
- evaluating the feature for the visited models
- approximating the distribution with the sample / calculating average

\[ P(F = f) = \sum_{F^G = f} P(G) \]
Basics of MCMC methods II.

- Ordering-based MCMC algorithm
  - Random walk in the space of variable orderings
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Summary
Fusion of factual knowledge and complex posteriors

- uncertain (statistical) inference
  - clinical/gene measurement data
- statistics of publications
- factual knowledge
  - ontologies
  - meta-data of publications (authors, publication year; concept occurrence)
Earlier works – first-order probabilistic logic

- distribution over possible worlds
- distribution over possible objects

Practical approaches:
- Knowledge-based model construction
- Relational Bayesian networks
- Bayesian logic programs
- Stochastic logic programs
- Bayesian logic
- Markov logic

- Overview
Probabilistic Annotated Bayesian Network Knowledge Bases (PABN-KBs)

Model elements:

- Bayesian networks
  - uncertain part
  - probabilistic relations

- Textual/xml annotations
  - basic description of entities
  - mapping model elements to „outer” knowledge sources

- Factual knowledge bases
  logical relations among objects

- Probabilistic knowledge base (pKB) \( P(G/D) \)
- Logic knowledge base (IKB) factual statements
The FOPL language

Language elements:

- Bayesian networks – possible worlds
- distribution over models
- factual knowledge sources

- predicates:
  - inherited from the factual part
  - dependence (structural) relations of model elements (nodes)

- logic operators
  - $\land, \lor, \neg, \exists, \forall$

- semantics (probability of a sentence):

$$p(\alpha \mid \mathcal{K}) = E_{p(M \mid \mathcal{K})}[\alpha^M] = \sum_{G : M(G) \in \mathcal{M}(\mathcal{K}^l)} \alpha^{M(G)} p(G \mid \mathcal{K})$$
A BN oriented FOPL language

Predicates about structural relations of nodes

- directed edge
- directed path
- MBM – Markov blanket membership

- parental set
- MB – Markov blanket set
- MBG – Markov blanket graph
A BN oriented FOPL KB

KB elements:

- set of Bayesian networks
- prior distribution over them
- annotations: nodes $\rightarrow$ ontology entities
  concepts in articles
- publication repository
- ontologies like GO
FOPL query examples

Basics:

„What is the Markov blanket of variable ‘X’?”

Involving annotations:

„What is the probability that the Markov blanket of ‘X’ will contain variables from a certain class?”

Involving the logic knowledge base:

„What is the probability that every concept in the Markov blanket of ‘X’ appears in one publication?”
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Feature subset selection and its generalizations I.

Feature subset selection (FSS)

- A relevant subset of features
- Two main approaches:
  1. Wrappers (score function)
  2. Filters (conditional distribution of target variables)
Feature subset selection and its generalizations II.

Feature Subgraph Selection (FSG)
- Identification of the relevant subgraph:
  - Relevant subset of features
  - Dependency between them

Most Probable Sentence (MPS)
- Not enough data to select a feature with a dominant posterior
- Multiple selection: K best features
The „Most Probable Sentences” problem

Given: a set of sentences of interest – target set

Task: find the N highest-scoring (those of highest probability) ones

E.g.: „find the N most probable MBM sets of variable X”
Search-and-estimate schemes

Exhaustive enumeration of DAGs:

- for each possible DAG: evaluate target sentences
- calculate the probability of each sentence on-the-fly (sum the probability of the models in which the sentence is true)

Theoretical solution used for testing
MCMC sampling

- MCMC random walk over DAGs
- for each visited DAG:
  - find true sentences / groundings
- update their probabilities:
  \[ P(S) = \frac{\#(G: KB^G \models S)}{\#(G)} \]

```python
listMPS = [];
while( ! MCMC.hasConverged() ){
    model = MCMC.nextModel();
    listNewS = PLEngine.evaluatePredicate(query, model);
    listMPS.insert(listNewS);
}
listMPS.orderBy(prob);
listMPS.truncate(N);
return listMPS;
```
The implemented framework

RESULTS

search
-and-
estimate
module

predicates
about models

truth
values

MCMC
engine

stored
samples

statistical
data

starting
model

GO
DB

PubMed
DB

SWI
Prolog
engine

Prolog/SQL
interface

MySQL
engine

wrapper

wrapper

GO
DB

PubMed
DB

logic knowledge bases (IKB)

pKB

pKB

theorem
prover

RESULTS
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Application domain – I. Rheumatoid arthritis

Statistical data:
- clinical observations
  - age, …
  - gender
  - received cures
- gene measurements:
  - single nucleotide polymorphisms (SNP)

Logic knowledge:
- SNP database
Application domain – II.
Genome Wide Association Studies

- moderate number of clinical variables (in the range of 50)
- hundreds of genotypic SNP variables for each patient
- thousands of gene expression measurements

E.g.: Asthma
- Complex disease mechanism
- Half of the patients do not respond well to current treatments
- Unknown pathways in the asthmatic process
The multilevel structure of GWAS

- SNPs
- Haplotype blocks
- Genes
- Proteins
- Pathways
- Clinical factors

Personalized medicine

Logical knowledge base

Haplotype prediction

Protein structure prediction

FOL-KB

IKB

pKB

statistical data
„What is the probability that a given SNP ‘X’ influences certain encoding genes $Y_1, Y_2$ that have an effect on certain symptoms of asthma $S_1, S_2, S_3$?”

„What is the probability that a SNP directly influences the structure of a certain protein, which modifies the „pathway” (the process of the disease), which in turn results in a change of the phenotype (some clinical variable)?”
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Goal:
Fusion of expertise, data and factual/textual domain knowledge within a first-order logic

Implemented:
Bayesian fusion of a complex posterior over BNs (causal models) and domain literature
Future work

- Extending the model representation
- Hierarchic Bayesian networks
- Describing priors by graph-grammars